Crystal Structure of the Antiestrogen [2-(4-Benzylphenoxy)ethyl]diethylammonium Chloride

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The crystal structure of [2-(4-benzylphenoxy)ethyl]diethylammonium chloride has been evaluated from the X-ray data collected at the X9B beam line from the very small crystal, of dimensions less than 5 μm. This compound is a diphenylmethane analog of the antiestrogen tamoxifen, which antagonizes the binding of histamine to intracellular growth-regulatory sites associated with antiestrogen binding in microsomes and nuclei. It enhances the therapeutic index of some chemotherapy drugs and has low toxicity to tissues like bone marrow, gut and hair. Due to these properties it is tested in a treatment of for metastatic prostate or breast cancer.

The stereochemistry of the molecule is close to that of clomiphene and tamoxifen. It is likely that the diphenylmethane moiety is responsible for the common antiestrogen properties of these molecules and the third phenyl ring, absent in the present compound, is involved in other antiproliferative actions of three-ring antiestrogens on cancer cells.